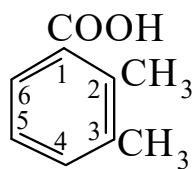




>>Entry Name: **2,3-Dimethylbenzoic acid**, 9CI, 8CI

Synonym(s): *vic-o*-Xylylic acid. Hemellitic acid



CAS Registry Number: 603-79-2

Molecular Formula: C₉H₁₀O₂

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 144°

pKa Value: pK_{a1} 3.72 (25°)

Other Data: Steam-volatile

Aldrich: 13815-0

Fluka: 39581

Rare Chemicals Library: S43043-9

>>Derivative: Me ester

CAS Registry Number: 15012-36-9

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Physical Description: Liq.

Boiling Point: Bp₁₂ 104-105°

>>Derivative: Chloride

CAS Registry Number: 21900-46-9

Molecular Formula: C₉H₉ClO

Molecular Weight: 168.622

Accurate Mass: 168.034192

Percentage Composition: C 64.11%; H 5.38%; Cl 21.02%; O 9.49%

Physical Description: Oil

Boiling Point: Bp₂₂ 128°

>>Derivative: Amide

CAS Registry Number: 5580-34-7

Molecular Formula: C₉H₁₁NO

Molecular Weight: 149.192

Accurate Mass: 149.084064

Percentage Composition: C 72.46%; H 7.43%; N 9.39%; O 10.72%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 155-156°

>>Derivative: Nitrile

Synonym(s): 2,3-Dimethylbenzonitrile. 1-Cyano-2,3-dimethylbenzene

CAS Registry Number: 5724-56-1

Molecular Formula: C₉H₉N

Molecular Weight: 131.177

Accurate Mass: 131.073499

Percentage Composition: C 82.41%; H 6.92%; N 10.68%

Physical Description: Oil

Boiling Point: Bp₁ 60-62°

Rare Chemicals Library: S44530-4

References: